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Role of Oxygen Vacancies and Surface Defects in Modulating Catalytic Activity of Mixed Transition Metal Oxides (MTMOs)

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Abstract: *Oxygen vacancies and other surface defects strongly influence the catalytic activity of mixed transition metal oxides (MTMOs) by altering local electronic structure, adsorption energetics, and reaction pathways. Here we quantify how vacancy formation energy, defect-induced electronic states, and local metal coordination modulate adsorption of key oxygen intermediates (O˙, OH˙, OOH˙) relevant for oxygen evolution/reduction and oxidation catalysis. Combining density functional theory (DFT) calculations, synthetic experimental trends, and simple microkinetic modeling, we show (i) a systematic correlation between vacancy formation energy and O˙ adsorption strength, (ii) how defect-stabilized mid-gap states tune electron transfer to adsorbates, and (iii) that an optimal (volcano-type) adsorption window exists where catalytic activity is maximized. We propose design rules for MTMOs to optimize vacancy concentration and local coordination to reach the adsorption optimum for desired reactions.*

Keywords*:* Mixed transition metal oxides, oxygen vacancies, surface defects, catalysis, DFT, adsorption energy, oxygen evolution reaction (OER), oxygen reduction reaction (ORR), vacancy formation energy